

A Global Equation-of-State Model for LLNL Applications

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Equation of state (EOS) models are crucial to developing a physics based understanding of many key materials properties that determine phase stability, pressure and temperature behavior, as well as dynamic phenomena. EOS models and experimental data are represented in practice by tables of thermodynamic variables pressure and energy as functions of temperature and density. The generation of accurate numerical EOS tables is a necessary requirement for the simulation of many kinds of high-energy dynamic processes, including explosive and impact loading of materials, shockwave propagation, inertial-confinement fusion, meteorite and comet impacts and planetary and stellar interior evolution. In these processes, matter experiences large ranges of temperature and density, with correspondingly large ranges of behaviors exhibited.

QEOS, developed and used at LLNL, is a global EOS model based on the Thomas-Fermi approximation for atoms. Molecular character is not inherently treated, although it is possible through existing code to consider molecular degrees of freedom and dissociation. QEOS, therefore, is capable of investigating not only solids but also molecular fluids and covalently bonded systems.

QEOS is generally fit to experimental shock compression EOS data although fitting other experimental data also helps improve the overall quality of the QEOS output. Other experimental data that have been used to fit QEOS include porous Hugoniot, high pressure isotherms, critical points, Gruneisen parameter and expansion isobars for solid and liquid materials.

Demand is increasing for improved accuracy in EOS tables so that hydrodynamic simulations can be as realistic as possible. Upgrading QEOS is a response to this demand and will keep QEOS in the forefront of material models.

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